Reacting flows and vortices

Sanaz Arabzade, (University of Toronto)
Anne Bourlioux(Universite de Montreal)
Alexandre Desfosses Foucault (Universite de Montreal)
Pierre Gauthier (Rolls-Royce Canada)
Apala Majumdar (Oxford)
Catherine Mavriplis (University of Ottawa)
Mario Morfin Ramirez (University of Toronto)
Stephen Peppin(Oxford)
Mary Pugh (University of Toronto)
Louis-Xavier Proulx (Universite de Montreal)
Tim Reis (Oxford)
Nasim Shahbazian (University of Toronto)

Problem Statement

- Rolls Royce interest: chemistry in gas turbine combustor
- Challenge: reliable prediction of CO, NO and other pollutants
- Huge computational challenge: direct simulation with detailed chemistry of reacting turbulent flow.
- Currently feasible: large eddy simulations with simplified chemistry
- Still needed: chemicals above, only available with detailed chemistry
- Strategy: some form of hybrid CFD/detailed chemistry computation

Hybrid approach considered by Rolls Royce

1. Use CFD package for large eddy simulation of the reactive Navier-Stokes model with simplified chemistry,
2. Time-average CFD output to create spatially-dependent but time–independent values for the velocity (u, v, w), temperature T, pressure p, carbon monoxide CO, nitric oxide NO, carbon dioxide CO2, water H20, and oxygen O2,
3. Post–proces time-averaged data to identify so called "vortices" (regions of space in which a fluid particle would spend a good chunk of time before leaving the region),
4. Compute in each region a "residence time", the spatial averages of CO, NO, CO2, H20, O2, the temperature, and the pressure, and the fluxes of these quantities between regions.
5. Pass these quantities, along with the geometry of the decomposition (which region abuts which) to a chemistry software Chemkin (detailed chemistry).

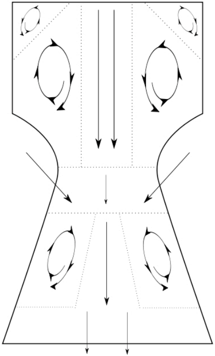
Hybrid approach considered by Rolls Royce - summary

In the procedure just described, a stiff PDE is handled in three stages:

1. the computation of a less-stiff PDE via CFD software (step 1),
2. the post-processing of the CFD solution (steps 2-4),
3. the computation of a detailed chemical network model via Chemkin (step 5).

Specific objective of working group

The working group has been asked to help with step 3: the segmenting of the fluid domain into subdomains that, in some way, correspond to largely-separate reaction chambers.



Approaches

A quick literature survey indicates a variety of existing methods for various applications. The group focussed on understanding and testing some of those existing classical or not-so-classical approaches.

1. *Greek* methods: Q-criterion, δ,λ_2, eigen helicity
2. critical points method
3. symbolic dynamic method
4. geometric methods
5. Haller's method (reference suggested by industrial partner)

Greek methods - general framework

Local vortex-identification criteria

Given the vector field $\vec{u} := (u(x,y), v(x,y))$ the deformation matrix

$$\nabla \vec{u} := \nabla \begin{pmatrix} u \\ v \end{pmatrix} = \begin{pmatrix} u_x & u_y \\ v_x & v_y \end{pmatrix}$$

is computed. This matrix is written in terms of its symmetric component and its antisymmetric component

$$\nabla \vec{u} = S + \Omega = \frac{1}{2}\left(\nabla \vec{u} + (\nabla \vec{u})^T\right) + \frac{1}{2}\left(\nabla \vec{u} - (\nabla \vec{u})^T\right) \quad (1)$$

Q criterion

The Q criterion segments the domain by identifying the points at which Ω is "bigger" than S as being points within a vortex and the points at which Ω is "smaller" than S as being points outside a vortex. Hunt et al. use the matrix norm

$$\|\Omega\|^2 := \mathrm{Tr}\left(\Omega\,\Omega^T\right) = \Omega_{11}^2 + \Omega_{12}^2 + \Omega_{21}^2 + \Omega_{22}^2.$$

That is, $\nabla\vec{u}$ is viewed as a vector in R^4 with the usual dot product. In this context, S and Ω are orthogonal.

$$S \in \mathrm{span}\left\{\begin{pmatrix}1\\0\\0\\1\end{pmatrix}, \begin{pmatrix}1\\0\\0\\-1\end{pmatrix}, \begin{pmatrix}0\\1\\1\\0\end{pmatrix}\right\} \quad \Omega \in \mathrm{span}\left\{\begin{pmatrix}0\\1\\-1\\0\end{pmatrix}\right\}$$

The Q criterion is then

$$\|S(x,y)\|^2 < \|\Omega(x,y)\|^2 \quad \Longrightarrow \quad (x,y) \text{ is in a vortex}$$

This can be written in terms of the matrix invariants, $\mathrm{Tr}(\nabla\vec{u})$ and $\mathrm{Det}(\nabla\vec{u})$:

$$\mathrm{Tr}(\nabla\vec{u})^2 - 2\mathrm{Det}(\nabla\vec{u}) < 0 \quad \Longrightarrow \quad (x, y) \text{ is in a vortex} \tag{2}$$

and

$$\text{incompressible flow and } \mathrm{Det}(\nabla\vec{u}) > 0 \quad \Longrightarrow \quad (x, y) \text{ is in a vortex} \tag{3}$$

Δ criterion

The Δ criterion identifies a vortex as a region where $\nabla\vec{u}$ has complex eigenvalues. For the 2-d flow, the eigenvalues of $\nabla\vec{u}$ are

$$\frac{1}{2}\mathrm{Tr}(\nabla\vec{u}) \pm \frac{1}{2}\sqrt{\mathrm{Tr}(\nabla\vec{u})^2 - 4\mathrm{Det}(\nabla\vec{u})}$$

If we compare the projection approach (now to be called the Q-criterion) to the eigenvalue approach (the Δ criterion)

$$\mathrm{Tr}(\nabla\vec{u})^2 - 4\mathrm{Det}(\nabla\vec{u}) < 0 \quad \Longrightarrow \quad (x, y) \text{ is in a vortex} \tag{4}$$

and

$$\text{incompressible flow and } \mathrm{Det}(\nabla\vec{u}) > 0 \quad \Longrightarrow \quad (x, y) \text{ is in a vortex} \tag{5}$$

λ_2 criterion

Jeong and Hussain proposed seeking minima of the pressure as a method for identifying vortices. Taking the gradient of the Navier–Stokes equations and writing it in terms of the matrices S and Ω yields

$$\frac{DS_{ij}}{Dt} - \nu S_{ij,kk} + \Omega_{ik}\,\Omega_{kj} + S_{ik}\,S_{kj} = -\frac{1}{\rho} p_{\,,ij}. \tag{6}$$

A local pressure minimum requires that the Hessian of p have two positive eigenvalues. If the flow is steady and the viscosity is zero then the Hessian of the pressure is simply $\Omega^2 + S^2$ and

$$\Omega^2 + S^2 \text{ has two negative eigenvalues} \quad \Longrightarrow \quad (x, y) \text{ is in a vortex} \tag{7}$$

Special cases: 2d incompressible flows

If the flow is incompressible then the eigenvalues of $\Omega^2 + S^2$ are $-\mathrm{Det}(\nabla \vec{u})$ with multiplicity two and so

$$\text{incompressible flow and } \mathrm{Det}(\nabla \vec{u}) > 0 \quad \Longrightarrow \quad (x, y) \text{ is in a vortex} \tag{8}$$

Hence the Q method, the Δ criterion, and the λ_2 method are identical for 2-d incompressible flows but could have different results for compressible flows.

Eigen helicity method

The Q, Δ, and λ_2 methods relied fully on the vorticity tensor Ω and the strain rate tensor S. However, eigenvectors of the strain rate tensor S do not necessarily align with the vortex tubes. This can lead to spurious predictions of the location of vortex boundaries.

Levy et al. introduced the Helicity method which uses the normalized helicity H_n to extract vortex core lines. H_n is the cosine of the angle between $\mathbf{v}$ and $\boldsymbol{\omega} = \nabla \times \mathbf{u}$

$$H_n = \frac{\mathbf{v} \cdot \boldsymbol{\omega}}{|\mathbf{v}||\boldsymbol{\omega}|}. \tag{9}$$

The sign of H_n indicates the direction of swirl (clockwise or anticlockwise) and the sign changes whenever there is a transition between primary and secondary vortices.

Zhang et al. propose a new scheme that presents a different alignment of the vorticity vector with the full eigen system of the velocity gradient tensor.
The quantity H_e is defined as follows.

$$H_e = \frac{\mathbf{n}_{swirl} \cdot \boldsymbol{\omega}}{|\mathbf{n}_{swirl}||\boldsymbol{\omega}|} \tag{10}$$

where $\mathbf{n}_{swirl} = -(\mathbf{e}_1 \times \mathbf{e}_2)i/2$, and $\mathbf{e}_1$ and $\mathbf{e}_2$ are the two eigenvectors corresponding to the complex conjugate eigenvalues of $\nabla\mathbf{u}$. By analogy with the Helicity method, the vortex core corresponds to regions where the magnitude of H_e is maximum.

Critical points methods

- critical point: vortex centre or saddle point?
- classification using the properties of critical point's Jacobian, ∇U which is defined as:

$$\begin{bmatrix} \frac{\partial u}{\partial x} & \frac{\partial u}{\partial y} \\ \\ \frac{\partial v}{\partial x} & \frac{\partial v}{\partial x} \end{bmatrix}$$

Calculating the negative trace q and determinant, r of this matrix:

$$q = -(\frac{\partial u}{\partial x} + \frac{\partial v}{\partial y}) \tag{11}$$

$$r = \frac{\partial u}{\partial x}\frac{\partial v}{\partial y} - \frac{\partial u}{\partial y}\frac{\partial v}{\partial x} \tag{12}$$

If $r < 0$ the point is a saddle point and if $r > \frac{q^2}{4}$ it is a vortex centre.

Symbolic dynamics method

- Given $u(x, y), v(x, y)$ and a grid decomposition of the domain, does some mass initially in one region end up in another region?
- With this information construct the connectivity matrix: $M(i, j) = 1$ if some of the gas in region i went into region j, and zero otherwise.
- $jth - column$ the entries with value 1 will tell us which regions send material into the jth region. (directed graph)
- $M^p(i, j)$ contains the number of paths of length p from region i into region j.
- Regions that receive more mass than others have larger column sums. Mass cycles will be detected as recurrences

For example:

$$M = \begin{pmatrix} 0 & 1 & 1 & 1 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 1 & 0 \\ 1 & 0 & 1 & 0 \end{pmatrix}, \; M^2 = \begin{pmatrix} 1 & 0 & 3 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 1 & 2 & 1 \end{pmatrix}, \; M^3 = \begin{pmatrix} 0 & 1 & 4 & 1 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 1 & 0 \\ 1 & 0 & 4 & 0 \end{pmatrix}$$

We can see a cycle in the entries $M(1,1)$ and $M(1,4)$ This cycle indicate the presence of a vortex.

The Algorithm:

First, locate the regions that are receiving more mass. We do this detection, we add up all the columns of the powers of the matrix. This will give us a function on the domain: for each element of the partition, the number of ways there are to send mass to that element in the number of iterations that we pick for our experiment. Call this function F

Second, having located these regions, we can build level sets in the following way:

1. Take the domain and color the local maximums of F with a dark shade.
2. Using M, look at the elements around that gave mass to this element of the partition and color them with a lighter shade.
3. Do the same for M^2 with a lighter shade.
4. Repeat this process for regions that were colored already.
5. If we find an element of the partition that is darker than the one we want to color, this means that this element gives more mass to another local maximum. So we have found a border between two vortexes.

Geometric methods

- Instead of physical quantities use geometric properties of curves such as streamlines and pathlines.
- Sadarjoen and Post have used the curvature centre method for vortex detection.
- Calculate curvature centre for different points on the streamlines.
- Vortex regions can be identified on this grid of curv. pts: curvature centre points accumulate in the center of vortices.
- This method would detect easily circular vortices.
- Limitations since centre points might spread out such as in the case of elliptic vortices.

Geometric methods - Advantages

- The algorithm is parameter-free.
- Arbitrary shaped vortex regions can be extracted.
- Vector fields with and without divergence can be handled alike.
- The method is grid-independent.

inputs: streamline tracing and critical points. Vortex regions are defined in the case of a divergence-free vector field as a union of closed streamlines winding around a common center.

The method applies a rotation matrix on the vector field. It then uses a loop which is a positively oriented closed streamline in the rotated vector field. Such a loop intersects the original vector field at a constant angle since rotating the vectors around that angle yields a vector field tangential to the loop.
Vortex region candidates which are extracted are bounded by loops that start and end at saddle points. Due to continuity, at least one saddle is included in the closure of a bounded region R_i. The vortex region candidates R_i are disjunct but may be nested.

Haller's methods

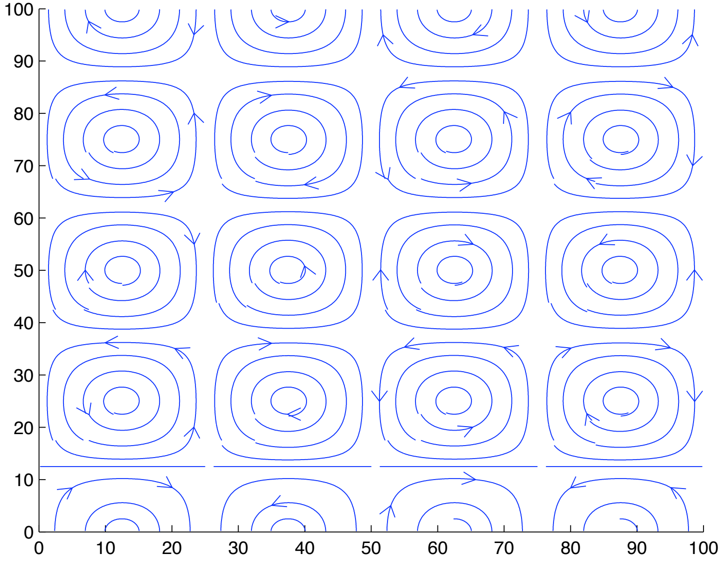
- Provides an "objective" definition of a vortex: one that does not depends on the frame of reference. A region that is labelled a "vortex" will still be labelled as such even if there's a change of coordinates: $\hat{x} = Q(t)x + b(t)$
- Although based on "Normal Hyperbolicity", it's not hard to code up.
- The method is defined for 3-d flows and reduces to 2-d flows in a natural manner.
- Unfortunately, the method does not generalise to compressible flows.

Test-cases

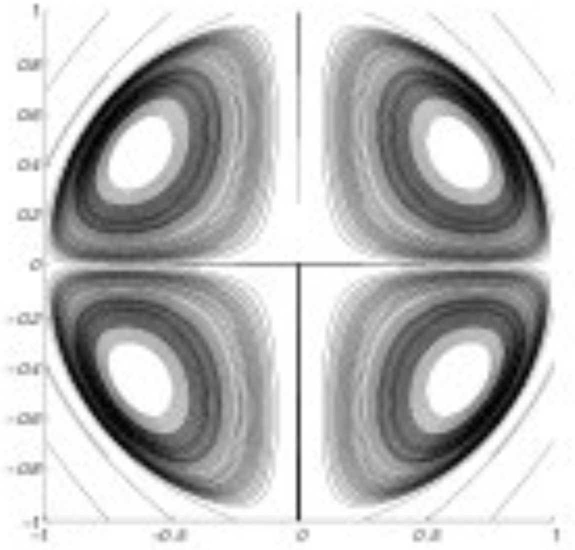
We focussed on 2-d (planar or axisymmetric) flows.

1. test-case 1: ABC flow: 2-D planar analytical solution of 2d Euler equations
2. test-case 2: Immersed droplet flow (test-case 1 in Haller's paper): analytical axisymmetric solution for Stokes equations
3. test-case 3: Driven cavity flow: direct numerical solution for 2d Navier-Stokes equations (downloaded from www.cavityflow.com)
4. test-case 4: Flow around a cylinder: Lattice-Boltzmann solution to 2d Navier-Stokes equations, computed by Tim Reis.

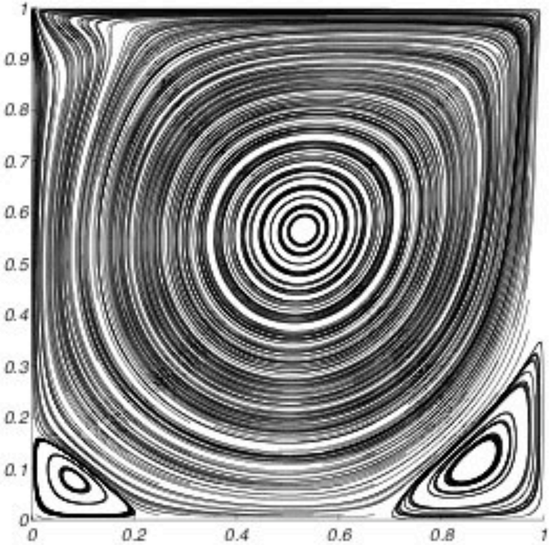
Test-case 1 : ABC flow



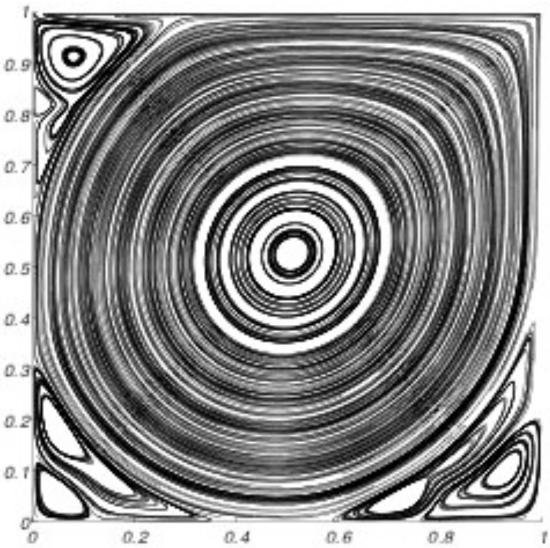
Test-case 2 : Immersed droplet flow



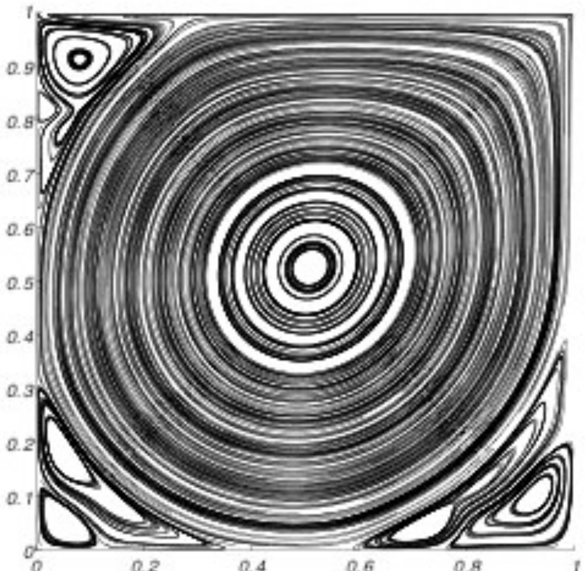
Test-case 3 : Driven cavity flow, a. Reynolds number=1000



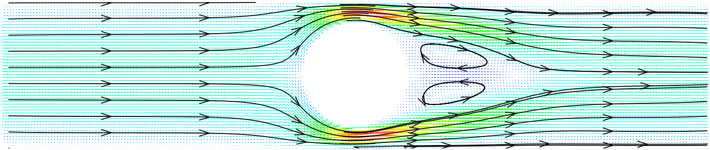
Test-case 3 : Driven cavity flow, b. Reynolds number=10000



Test-case 3 : Driven cavity flow, c. Reynolds number=20000



Test-case 4 : Flow around a cylinder



Results - Greek- Q criterion

Note: For 2d flows: identical results from other classical greek approaches.

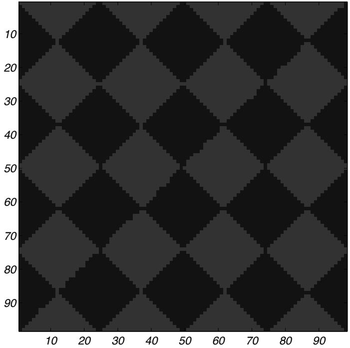


Figure: Q-criterion, ABC flow.

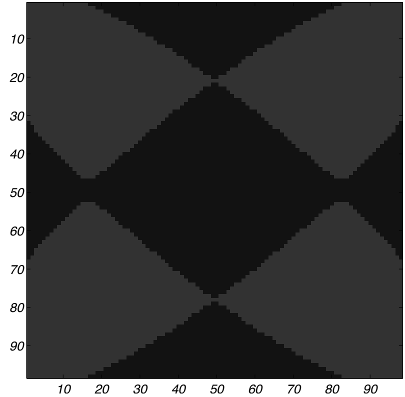


Figure: Q-criterion, Immersed drop.

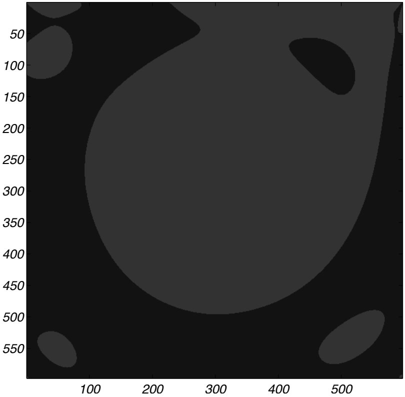


Figure: Q-criterion, driven cavity, Re=1000.

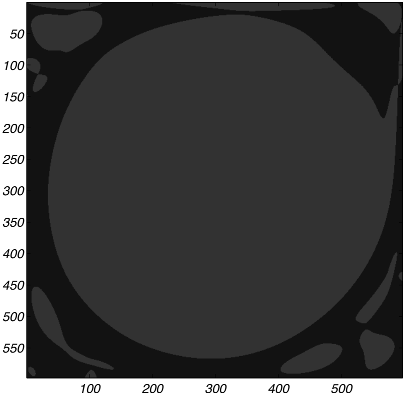


Figure: Q-criterion, driven cavity, Re=10000

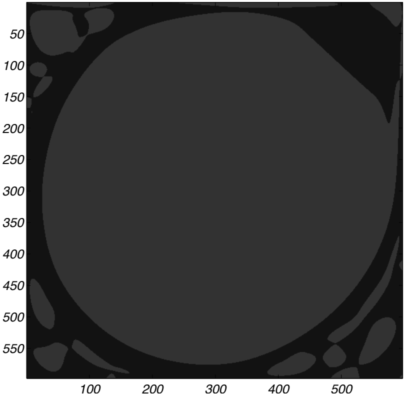


Figure: Q-criterion, driven cavity, Re=20000.

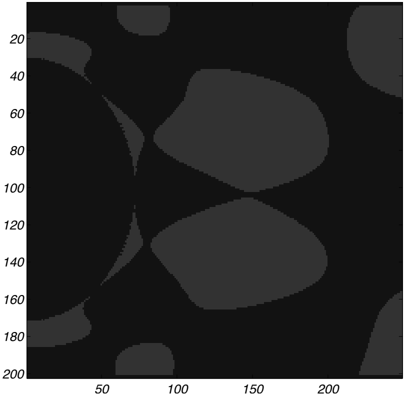
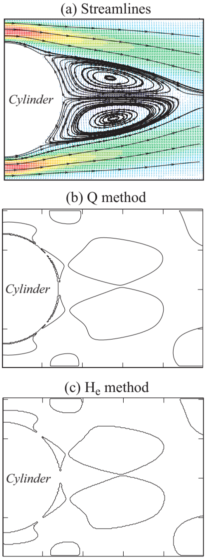


Figure: Q-criterion, Rolls-Q.

Results: comparison Q-criterion and eigen-helicity



We see that the Q-method and the H_e method qualitatively identify the vortex regions. They also omit parts of the vortex regions and also identify certain vortex-free regions as being vortices in some cases. It is disappointing to find that we do not get better results with the H_e-method. One possible improvement is to use a normalized version of the Eigen Helicity as shown below -

$$H_e^* = \frac{|H_e|^2}{\max\left\{|H_e|^2\right\}} \tag{13}$$

which takes values in the range $[0, 1]$. The vortices correspond to the points $H_e^* = 1$ and one could use the threshold value $H_e^* = 0.95$ to trace the boundaries of the vortex regions

Results - critical points

The method is applied to a 2D cavity driven flow. The zero-contour lines of u and v intersect within the potential cell showing the critical point is located inside the cell (Figure 1).

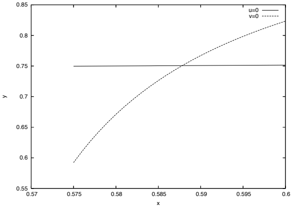


Figure: Critical point's location in the potential cell.

Applying the method, the location of the vortex centre is obtained inside the domain as shown in figure 2.

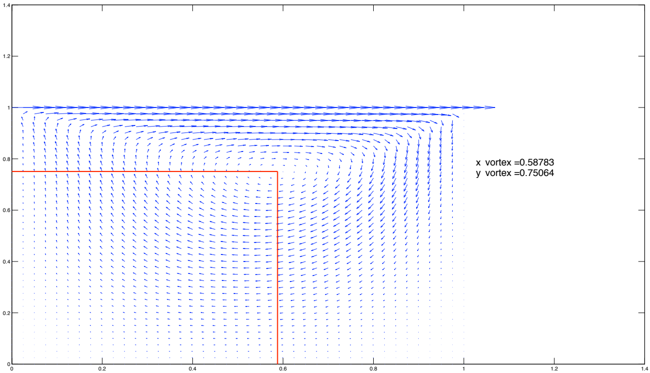


Figure: Centre of the vortex in the flow vector field.

Results - geometric

(Note: Published results, not implemented by working group.)
Here are two figures using the boundary loop and the λ_2 methods to detect vortrices for time-dependent simulation of the Kármán vortex behind a cylinder.

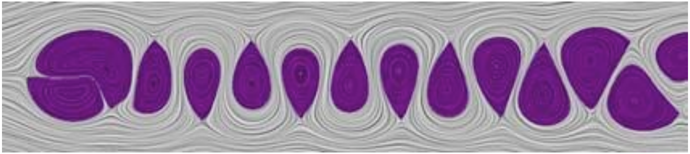


Figure: Boundary Loop method

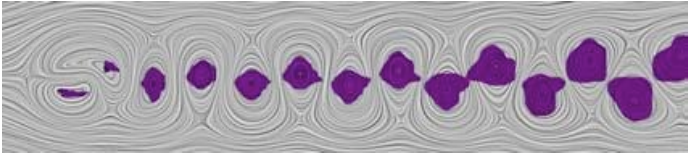


Figure: λ_2 method

Conclusions

- cheap and easy classical methods can get gross map of recirculating regions
- these have been tested on simple 2d synthetic and classical flows
- we foresee problems though with more arbitrary cases
- the predicted zones are not well delineated however
- thresholding did not improve the results
- perhaps Haller's method should be programmed
- recommend combining this method with other diagnostics or min flux identification or with avg Temp and mixture fraction as was done previously
- given the other approximations of this process this may be adequate
- Most of these methods are extendable to 3D and compressibility

Further work and recommendations

- either implement the Haller method (if easily tractable)
- or combine these methods with a technique to separate the recirculation regions based on:
  - a crude expansion of the identified regions perhaps using some diagnostic based on local velocities
  - a technique to find the "dividing" streamline between the regions by - identifying either a no or low normal flux line (streamline) - or identifying a line along which the curl of neighbouring velocities is zero (parallel) and the scalar product is negative (opposite directions) [This would only cover cases of abutting recirculation zones of opposite direction - which happens often but not exclusively].
  - some existing method (that we could not find but think must exist) to find a trough on a topological map. Basically this operation would be to calculate the path of lowest flux (or equivalently the locus of local minima).
- look at how meteorologists divide streamlines?

Further work and recommendations- 2

- fluxes between the regions would be easy with the CFD software if it is indeed flux-based
- Residence times are also assumed to be calculated as in the previous Rolls Royce work.
- it would be interesting to check the impact of switching the order of the zone-extraction post-processing and the time-averaging of the CFD data - due to reaction nonlinearities, output from Chemkin might be very sensitive to the ordering.